Impact of Optical Modes on the Pairing Potential in Bilayer Cuprates

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Superconducting transition temperature is calculated for differently doped bilayer cuprates. Superexchange is assumed to be the dominating mechanism of high-temperature superconductivity, but the contribution from the phonon potential is not negligible, which qualitatively explains the observed weak isotopic effect. The calculated value $2\Delta_{max}/k_BT_C \simeq 4.5$ is close to the experiment in the case of optimum doping.

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I. INTRODUCTION

The High Temperature Superconductivity (HTSC) was discovered 11 years ago. None of the proposed HTSC mechanisms has been commonly accepted yet (see [1]). Unlike the case in normal low-temperature superconductors, the energy gap in HTSC materials is different at different points of the Brillouin zone. This dependence is important, for the understanding of the HTSC mechanism.

In [2,3] we found solutions of the Bardeen-Cooper-Schrieffer (BCS) equations taking copper spin superexchange into consideration. This interaction was found to lead to a reasonable critical temperature T_C and d-symmetry of the energy gap in superconducting cuprates. The conclusion about the d-symmetry of the order parameter was confirmed by recent studies of photoemission spectra [4]. In the present work we additionally consider the electron - phonon interaction with optical buckling A_{1g}, B_{1g} and breathing A_g, E_g modes to explain the weak isotope effect in these compounds.

II. POTENTIAL OF CURRENT CARRIERS PAIRING THROUGH OPTICAL BUCKLING AND BREATHING MODES

In the compound $YBa_2Cu_3O_{7-x}$ holes interact most strongly with an electric field perpendicular to the CuO_2 plane. This field is mainly induced by triply charged yttrium ions [5]. The operator of binding energy with oscillations perependicular to the CuO_2 plane has the form

$$H_{h-ph} = e\sum_{n\sigma}\left\{\mathbf{E}_x\mathbf{u}_x\left(a\mathbf{n}+\frac{a\mathbf{x}}{2}\right)p^{\sigma\sigma}_{nx}+\mathbf{E}_y\mathbf{u}_y\left(a\mathbf{n}+\frac{a\mathbf{y}}{2}\right)p^{\sigma\sigma}_{ny}\right\}, \quad (1)$$

where $p^{\sigma\sigma}_{nx}$ and $p^{\sigma\sigma}_{ny}$ are the Hubbard operators of oxygen holes, $\mathbf{u}_x(n)$ and $\mathbf{u}_y(n)$ are the displacements vectors of O(2) and O(3) positions in a unit cell with the number n, $\mathbf{x}$ and $\mathbf{y}$ are unit vectors of the axes a and b respectively, a is the lattice constant, and $E_x = 1.2\cdot10^8$ V·cm^{-1}, $E_y = 1.5\cdot10^8$ V·cm^{-1} are the components of electric field along the the axis c, calculated in [6]. For simplicity, we put $E = E_x = E_y = 1.35\cdot10^8$ V·cm^{-1}. Then, calculating the commutator $\left[\Psi^{\downarrow,pd}_{\mathbf{k}}, H_{h-ph}\right]$ and using the expression

$$\left[\Psi_{\mathbf{k}}^{\downarrow,pd}, H_{h-ph}\right] = \sum_{\alpha,\mathbf{q}} V^{\alpha}(\mathbf{q})\Psi_{\mathbf{k}-\mathbf{q}}^{\downarrow,pd}(b_{\mathbf{q}} + b_{-\mathbf{q}}^{+}),$$

where $\Psi_{\mathbf{k}}^{\downarrow,pd}$ is the quasiparticle operator of singlet-correlated oxygen holes, $b_{-\mathbf{q}}^{+}$ and ($b_{\mathbf{q}}$ are the phonon creation and annihilation operators, one finds

$$V^{\alpha}(\mathbf{q}) = \frac{e}{2}E\sqrt{\frac{\hbar}{2m\omega_{\alpha}}}\left[\cos\left(\frac{q_x a}{2}\right) \pm \cos\left(\frac{q_y a}{2}\right)\right], \tag{2}$$

where $\omega_{\alpha} = \omega_{\mathrm{A}_{1g}}$ =440 cm^{-1} and $\omega_{\mathrm{B}_{1g}}$ =340 cm^{-1} [7]. The plus and minus signs correspond to the modes A_{1g} and B_{1g} respectively, e is the electron charge, and m is the mass of the unit cell. Since the difference between $\omega_{\mathrm{A}_{1g}}$ and $\omega_{\mathrm{B}_{1g}}$ is not so important, they are put equal to ω_{G} =400 cm^{-1}.

Using the Frohlich procedure, the potential of current carriers interating through the phonon field of buckling modes A_{1g} and B_{1g} is written as

$$G(\mathbf{k}' - \mathbf{k}) = 2G_0^2\frac{1 + \frac{1}{2}\left[\cos\left(k_x' - k_x\right)a + \cos\left(k_y' - k_y\right)a\right]}{\left(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}\right)^2 - \left(\hbar\omega_G\right)^2}\hbar\omega_G, \tag{3}$$

where $G_0 = 35$ meV.

Assuming that the constant of interaction with the modes A_g and E_g (and their frequencies) are identical, the contribution to the pairing potential is written as

$$B(\mathbf{k}' - \mathbf{k}) = 2B_0^2\frac{1 - \frac{1}{2}\left[\cos\left(k_x' - k_x\right)a + \cos\left(k_y' - k_y\right)a\right]}{\left(\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}\right)^2 - \left(\hbar\omega_B\right)^2}\hbar\omega_B. \tag{4}$$

According to the estimate of [8], the constant B_0 is about 60 meV. The frequencies ω_{A_g} and ω_{E_g}, taken from [9], are about 480 cm^{-1}.

III. EQUATION FOR THE GAP

The BCS equation for the energy gap, taking into account the interaction via the phonon field and the superexchange between copper spins, has the form

$$\Delta_{\mathbf{k}'} = \sum_{\mathbf{k}}\left\{P^2\left[G(\mathbf{k}' - \mathbf{k}) + B(\mathbf{k}' - \mathbf{k})\right]\theta(\hbar\omega_D - |\varepsilon_{\mathbf{k}'} - \varepsilon_{\mathbf{k}}|) - J^{dd}(\mathbf{k}' - \mathbf{k})\right\}\left\langle\Psi_{\mathbf{k}}^{\downarrow,pd}\Psi_{-\mathbf{k}}^{\uparrow,pd}\right\rangle, \tag{5}$$

where $J^{dd}(\mathbf{q})$ is the Fourier transform of the superexchange parameter $J = 57$ meV,

$$J^{dd}(\mathbf{q}) = 2J\left(\cos q_x a + \cos q_y a\right),$$

$\omega_D = 500$ cm^{-1} is the Debye frequency, and $P = \frac{1}{2}(1 + x)$. The correlation function is given by

$$\left\langle\Psi_{\mathbf{k}}^{\downarrow,pd}\Psi_{-\mathbf{k}}^{\uparrow,pd}\right\rangle = -\frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}\tanh\left(\frac{E_{\mathbf{k}}}{2k_BT}\right),$$

where $E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2}$. The chemical potential μ and the hole concentration x for two copper sites in the bilayer (assuming that the antibonding band is ampty) are related as

$$x = P\sum_{\mathbf{k}}\left[\exp\left(\frac{\varepsilon_{\mathbf{k}} - \mu}{k_BT}\right) + 1\right]^{-1}.$$

At $x = 0.33$ the chemical potential is placed on 10 meV below the saddle singularity peak in the density of states. The dispersion $\varepsilon_{\mathbf{k}}$ is chosen as

$$\varepsilon_{\mathbf{k}} = P\left[2t_1\left(\cos k_x a + \cos k_y a\right) + 4t_2\cos k_x a\cos k_y a + 2t_3\left(\cos 2k_x a + \cos 2k_y a\right)\right], \tag{6}$$

where t_1, t_2, and t_3 are the effective hopping integrals. All the calculations are carried out at $t_1 = 70$ meV, $t_2 = 0$, and $t_3 = 5$ meV.

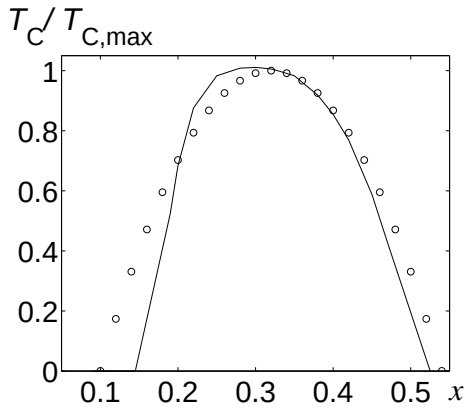

FIG. 1. Temperature dependence of the superconducting transition temperature in $YBa_2Cu_3O_{7-y}$ with doping: solid line (calculations) and the experimental points are sketched by open circles.

Figure 1 shows the dependence of the superconducting transition temperature of $YBa_2Cu_3O_{7-y}$ with doping. It is evident that the calculations qualitatively conform with the experimental data (normalized by the expression $T_C/T_{C,max} = 1 - 82.6(x - 0.32)^2$ [10]). However, their noncoincidence remains unexplained. Numerical solution of the energy gap equation yields a d-type symmetry of the order parameter $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x a - \cos k_y a)$ and a nonstandard value of $2\Delta_{max}/k_B T_C \approx 4.5$ with the superconducting transition temperature $T_{C,max} \sim 100$ K. Note that solutions of (5) with $J = 0$ lead to the s-type symmetry of the gap, $\Delta_{\mathbf{k}} = \Delta_0(\cos k_x a + \cos k_y a)$. The conclusion of [11] that the d-symmetry of the gap arises from pairing only through optical buckling modes seems to be groundless.

IV. CONCLUSION

Self-consistent solutions of the BCS gap equation are found in the class of short-range pairing potentials for various chemical potentials. When the Fermi level ε_F is near the bottom(top) of the band, the solutions correspond to the s-type pairing, while for ε_F in the center of the band the solution are related to the d-type. The short-range potentials considered are (i) superexchange interaction, (ii) interaction of current carriers via optical oscillations, and (iii) breathing and buckling modes of oxygen atoms in CuO_2 planes. The superconducting transition temperature is calculated for various oxygen indices x.

The dominant HTSC mechanism is a superexchange. However, the contribution of the phonon pairing is not negligible, that qualitatively explains the observed weak isotope effect. The calculated value $2\Delta_{max}/k_B T_C \approx 4.5$ is close to the experiment.

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